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Semi-classical correspondence and exact results : the case of the spectra of homogeneous Schrödinger operators (*)

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Résumé. — La méthode semi-classique BKW est susceptible en toute généralité de produire des résultats exacts. Ceux-ci, dans le cas de l'opérateur de Schrödinger avec potentiel homogène q^{2M}, prennent la forme d'une équation fonctionnelle pour le déterminant de Fredholm, ou bien d'identités arithmétiques satisfaites par la fonction Zeta du spectre.

Abstract. — The semi-classical WKB method is liable to yield exact results in full generality. Such results, in the case of the Schrödinger operator with a homogeneous potential q^{2M}, appear as a functional equation obeyed by the Fredholm determinant, or as arithmetical identities satisfied by the Zeta function of the spectrum.

We consider the following Schrödinger equation on the real axis :

$$\left(-\frac{d^2}{dq^2} + q^{2M}\right)\psi = \lambda\psi \qquad (M \text{ positive integer}) \tag{1}$$

and we start more specifically with the case $M = 2$ (homogeneous quartic oscillator).

From the eigenvalue spectrum $\{\lambda_n\}_{n\in\mathbb{N}}$ of equation (1), we build an entire function, the Fredholm determinant $\Delta(\lambda)$, and a meromorphic function, the Zeta function $\zeta(s)$:

$$\Delta(\lambda) = \prod_0^\infty (1 - \lambda/\lambda_n), \qquad \zeta(s) = \sum_0^\infty \lambda_n^{-s}. \tag{2}$$

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Analytic properties and some exact results concerning those functions already appear in [1-3] (all results quoted as known are drawn from [2] unless stated otherwise, but the Zeta function defined in [2] equals $C^{-4s/3}\,\zeta(s)$ where $C = \Gamma(1/4)^2(2/\pi)^{1/2}/3$, due to a different normalization of the spectrum). One interest of such results is to extend classical formulas of analysis : in the case $M = 1$ (harmonic oscillator) the spectrum consists of the positive odd integers and the Zeta function becomes $(1 - 2^{-s})$ times the Riemann Zeta function [4].

This note presents a *new* class of exact results that we have drawn from the semi-classical correspondence between the quantal equation (1) and the classical motion governed by the Hamiltonian $(p^2 + q^{2M})$. This correspondence is usually exploited to build asymptotic expansions of the spectrum for $\lambda \to \infty$ through the WKB method. The divergence of the resulting series [5] strengthens the belief that the semi-classical approach is doomed to be approximate. But this is not the case, as the mere extension of the WKB method to complex variables [6] actually gives control over the summability of semi-classical expansions by the Borel procedure [7], thus giving rise to certain exact analytical results. For instance, we have found that the determinant $\Delta(\lambda)$ for $M = 2$ satisfies the functional equation (where $j = e^{2i\pi/3}$) :

$$4\,\Delta(\lambda)\,\Delta(j\lambda)\,\Delta(j^2\,\lambda) = \Delta(\lambda) + \Delta(j\lambda) + \Delta(j^2\,\lambda) + 1 \tag{3}$$

of which we see no other direct proof (the same calculation for $M = 1$ would restore the reflection formula for the Euler Gamma function).

Since our derivation of (3) is lengthy [7] and relies at a point on a yet unproved regularity property, a direct check of (3) is desirable to confirm the validity of our approach, which could then find numerous applications in physics. Since equation (3) arises by the Borel resummation of a divergent series around $\lambda = \infty$, a reasonable test is to reexpand it around $\lambda = 0$ using the following obvious Taylor series, convergent for $0 \leqslant |\lambda| < \lambda_0$:

$$\log \Delta(\lambda) = -\sum_{n=1}^{\infty} \zeta(n)\,\lambda^n/n\,. \tag{4}$$

It then follows that equation (3) identifies each $\zeta(3\,n)$ to a polynomial in the $\zeta(k)$ $(1 \leqslant k < 3\,n)$; this polynomial is homogeneous of degree $3\,n$ if $\zeta(k)$ is assigned the degree k. For instance :

$$\zeta(3) = \frac{1}{6}\,\zeta(1)^3 - \frac{1}{2}\,\zeta(1)\,\zeta(2) \tag{5}$$

$$\zeta(6) = \frac{41}{3\,240}\,\zeta(1)^6 - \frac{11}{216}\,\zeta(1)^4\,\zeta(2) + \frac{1}{72}\,\zeta(1)^2\,\zeta(2)^2 + \frac{1}{24}\,\zeta(2)^3 + \frac{1}{4}\,\zeta(1)^2\,\zeta(4) - \frac{1}{4}\,\zeta(2)\,\zeta(4) - \frac{2}{5}\,\zeta(1)\,\zeta(5) \tag{6}$$

The annexed table, computed by the numerical method of reference [2], agrees perfectly with the latter formulas for $M = 2$. Remark : as

$$\zeta(1) = (8\,\pi^2)^{-1}(3/2)^{2/3}\,\Gamma(1/3)^5 \tag{7}$$

and as $\zeta(2)$ is the sum of a generalized hypergeometric ${}_5F_4$ series (a result found jointly with D. and G. Chudnovsky [3]), equation (5) constitutes a closed analytical expression for $\zeta(3)$ in the case $M = 2$.

To extend our results to arbitrary $M > 2$, it is useful to redefine the determinant as :

$$D(\lambda) = e^{-\zeta'(0)}\,\Delta(\lambda) = \exp\left(-\zeta'(0) - \sum_{1}^{\infty} \zeta(n)\,\lambda^n/n\right) \tag{8}$$

Table I

$M = 2$		
n	$\zeta(n)$	$\zeta^P(n)$
1	2.289908804320	0.763302934770
2	0.996320827679	0.833155797907
3	0.860517138943	0.822472813464
4	0.796211192704	0.786494804331
5	0.747295110967	0.744760013169
6	0.703855987715	0.703190573374

$M = 3$		
n	$\zeta(n)$	$\zeta^P(n)$
1	1.721346195	0.713004939
2	0.838749154	0.718952295
3	0.680579268	0.655376819
4	0.585204245	0.579516165
5	0.509234298	0.507930487
6	0.444390836	0.444090783

and to consider jointly the alternating determinant and Zeta functions, which arise naturally through the reflection symmetry of the even potential q^{2M} [2] :

$$\left.\begin{aligned} \zeta^P(s) &= \sum_0^\infty (-1)^n \lambda_n^{-s} \\ \Delta^P(\lambda) &= \prod_0^\infty (1 - \lambda/\lambda_{2n})(1 - \lambda/\lambda_{2n+1})^{-1} \end{aligned}\right\} \tag{9}$$

$$= \exp\left(-\sum_1^\infty \zeta^P(n)\,\lambda^n/n\right) \qquad (|\lambda| < \lambda_0). \tag{10}$$

The WKB analysis of a Borel transform of $\Delta^P(\lambda)$ around $\lambda = \infty$ likewise leads to the functional relations :

$$\left.\begin{aligned} &\frac{\Delta^P(e^{2\pi i\mu}\lambda)}{\Delta^P(e^{-2\pi i\mu}\lambda)} = e^{2\pi i\mu - 2i\varphi(\lambda)} \qquad (\mu \equiv [2(M+1)]^{-1}) \\ &\varphi(\lambda) \equiv \operatorname{Arc\,sin}\{[D(e^{2\pi i\mu}\lambda)\,D(e^{-2\pi i\mu}\lambda)]^{-1/2}\} \end{aligned}\right\}. \tag{11}$$

The functional equation for $D(\lambda)$ itself is now just a consistency condition for the system (11) written for λ, $e^{4\pi i\mu}\lambda$, etc... :

$$\sum_{k=0}^{M} \varphi(e^{4\pi i k\mu}\lambda) = \pi/2 \tag{12}$$

(this could also be rewritten as a polynomial in the D's).

Now the expansion of (11) around $\lambda = 0$ yields :

— at zeroth order : the relation $\varphi(0) = \pi\mu$, which restores a known result :

$$e^{-\zeta'(0)} = D(0) = (\sin \pi\mu)^{-1} \tag{13}$$

— at any higher order n, an expression for

$$\operatorname{cotg} \pi\mu . \sin 2\pi n\mu\zeta^P(n) - \cos 2\pi n\mu\zeta(n) \tag{14}$$

as a polynomial either in the $\zeta(k)$ alone or (at one's choice) in the $\zeta^P(k)$ alone, for $k < n$ (those polynomials being homogeneous of degree n under the previous convention). When n is a multiple of $(M + 1)$, $\zeta^P(n)$ disappears from the left hand side which then only contains $\zeta(n)$, and *vice versa* when M *and* $2\,n/(M + 1)$ are odd integers. The first relations read :

$$\operatorname{cotg} \pi\mu . \sin 2\,\pi\mu\zeta^P(1) - \cos 2\,\pi\mu\zeta(1) = 0 \quad \text{(already known)} \tag{15}$$

$$\operatorname{cotg} \pi\mu . \sin 4\,\pi\mu\zeta^P(2) - \cos 4\,\pi\mu\zeta(2) = [2 \cos \pi\mu\zeta^P(1)]^2 \tag{16}$$

$$\operatorname{cotg} \pi\mu . \sin 6\,\pi\mu\zeta^P(3) - \cos 6\,\pi\mu\zeta(3) = 4 \cos^2 \pi\mu[3 \cos 2\,\pi\mu\zeta^P(1)\,\zeta^P(2) - 2 \cos^2 \pi\mu\zeta^P(1)^3] . \tag{17}$$

We have checked numerically several of the relations (16-17) and following, up to $M = 4$. The explicit formulas known for $\zeta(2\,n)$ and $\zeta^P(2\,n + 1)$ in the harmonic case [4] ($M = 1$), as well as equations (5-6) for $M = 2$, are just special instances of those (the existence of such relations also suggests that the spectrum of equation (1) has rich arithmetical properties).

Our results confirm that the complex WKB method can be implemented in an exact form for analytic potentials in one degree of freedom. Applied to the inhomogeneous anharmonic oscillator $(- \mathrm{d}^2/\mathrm{d}q^2 + \kappa q^2 + q^4)$ as our last example, it leads to a generalization of (3) :

$$D(\lambda, \kappa)\, D(j\lambda, j^2\, \kappa)\, D(j^2\, \lambda, j\kappa) = D(\lambda, \kappa) + D(j\lambda, j^2\, \kappa) + D(j^2\, \lambda, j\kappa) + 2\,, \tag{18}$$

with definition (8) for D. It seems however more difficult to extract from (18) than from (3) *numerical* formulas that would be at the same time exact and interesting.

Another still harder problem would be to see how much of this exact approach persists in the case of several degrees of freedom (possibly nothing for a non-integrable system).

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